New high-pressure phase of Al_2O_3 and implications for Earth's D" layer.

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Alumina (Al_2O_3) is an important ceramic material and a major component of the Earth's mantle. According to theoretical [e.g., 1] and experimental [e.g., 2] studies, above 80 GPa corundum transforms into the Rh_2O_3(II)-type structure, and it was expected [1] that above 200 GPa a perovskite-type phase becomes stable.

Using *ab initio* simulations (we have calculated the full *P-T* phase diagram) and high-pressure experiments, we show that a $CaIrO_3$-type phase, isostructural with the post-perovskite phase of $MgSiO_3$ [3,4] becomes stable above 130 GPa. This necessitates a re-interpretation of previous shock-wave experiments [4], and has important implications for the use of alumina in high-pressure experiments. High electrical conductivity of the $CaIrO_3$-type phase of Al_2O_3 suggests an explanation for the high electrical conductivity of the D'' layer of the Earth, dominated by the $CaIrO_3$-structured phase of magnesium silicate. We show that incorporation of Al into $MgSiO_3$ shifts the perovskite/post-perovskite equilibrium to higher pressures, but this is more than compensated by the opposite effect of Fe^{2+} and Fe^{3+} (Ref. 6) at mantle compositions.

References:

[1] Thomson K.T., Wentzcovitch R.M., Bukowinski M.S.T. (1996). *Science* **274**, 1880-1882.
[2] Lin J.F., et al. (2004). *Nat. Mater.* **3**, 389-393.
[3] Oganov A.R., Ono S. (2004). *Nature* **430**, 445-448.
[4] Murakami M., et al. (2004). *Science* **304**, 855-858.
[5] Weir S.T., Mitchell A.C., Nellis W.J. (1996). *J. Appl. Phys.* **80**, 1522-1525.
[6] Ono S., Oganov A.R., Ohishi Y. (2004). Submitted.